

Ising-XY Transition in Three-dimensional Frustrated Antiferromagnets with Collinear Ordering

A.O. Sorokin^{1,2*}

¹*Department of Physics, St. Petersburg State University, 198504 St. Petersburg, Russia and*

²*Petersburg Nuclear Physics Institute, NRC Kurchatov Institute, 188300 St. Petersburg, Russia*

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Using Monte Carlo simulations, we study the critical behavior of two models of frustrated XY antiferromagnets with a collinear spin ordering and with an additional twofold degeneracy of the ground state. We consider a classic antiferromagnet on a body-centered cubic lattice with an additional antiferromagnetic exchange interaction between next-nearest spins, and a ferromagnet with an extra antiferromagnetic intralayer exchange. In both models, a single first-order transition on the discrete and continuous order parameters is found. Observed critical pseudo-exponents are in agreement with exponents of XY magnets with a planar spin ordering like a stacked-triangular antiferromagnet and helimagnets belonging to the same symmetry class.

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I. INTRODUCTION

Critical phenomena in frustrated magnetic systems are very attractive due to realization in them a plurality of symmetry breaking scenarios [1]. During the last several decades, it have been discussed a possibility that the new universality class different from the class of the usual $O(N)$ model is realized in magnets with planar spin ordering like a stacked-triangular antiferromagnet (STA) and helimagnets [2]. In such systems, the $O(N)/O(N-2)$ symmetry is broken, whereas in the $O(N)$ model the broken symmetry is $O(N)/O(N-1)$. In the case of XY spins ($N = 2$) and a planar ordering, the broken $O(2) = \mathbb{Z}_2 \otimes SO(2)$ symmetry relates to global spin rotations and inversions. In three-dimensional systems belonging to the later symmetry class, one observe a single fluctuation-induced first-order transition describing by the Ginzburg-Landau functional (the $O(N) \otimes O(2)$ -model)

$$F = \int d^3x \left((\partial_\mu \phi_1)^2 + (\partial_\mu \phi_2)^2 + r(\phi_1^2 + \phi_2^2) + u(\phi_1^2 + \phi_2^2)^2 + 2w((\phi_1 \phi_2)^2 - \phi_1^2 \phi_2^2) \right), \quad (1)$$

where $\phi_{1,2}$ are two-component vectors, $u, w > 0$ and $u > w$. This transition is close to a second-order transition, therefore at the critical point, one may observe (pseudo) scaling behavior and universality. Such an imitation of a second-order transition behavior is typical for weak first-order transitions, e.g. as in the two-dimensional 5-state Potts model [4].

In terms of the renormalization group (RG) [5, 6], the fixed point in the model (1), being stable for large N , becomes complex-valued for the case $N = 2$, with the small imaginary part. On the real part of the RG-diagram in a vicinity of this fixed point, the region exists where

the RG-flow is slow. It leads to imitation of the scaling behavior. This region is attractive in sense that trajectories starting from a sufficiently wide area of initial point cross it. The studies of the model (1) at $N = 2$ [5, 6] have shown that the region of the significant RG-flow slowdown is quite large, so one may observe a wide scatter of critical pseudo-exponents values for different lattice models. Furthermore, some models from considered symmetry class have a distinct first order of a transition (see, e.g. [7]).

In this work, we consider two models of frustrated XY antiferromagnets with a *collinear* spin ordering and with an additional broken \mathbb{Z}_2 subgroup of a lattice symmetry, so the full broken symmetry is also $\mathbb{Z}_2 \otimes SO(2)$. The first model is an antiferromagnet on a body-centered cubic lattice with an extra antiferromagnetic exchange interaction between next-nearest spins. This model is equivalent to two interacting antiferromagnetic sublattices. Due to competing of exchanges, the additional twofold degeneracy of the ground state appears [8]. Note that models of classic XY antiferromagnets with competing exchanges have been investigated for other lattices, e.g. a simple cubic [9], a face-centered cubic [10], a hexagonal closed-packed [11], and a stacked-triangular [12] lattices. For these models, an extra degeneracy of a ground state is threefold, and a transition of distinct first order occurs with breaking of the $\mathbb{Z}_3 \otimes SO(2)$ symmetry.

The second model is so-called stacked-J₁-J₂ model of a ferromagnet on a simple cubic lattice with an additional intralayer exchange, where we have a twofold degeneracy of the ground state [13]. This model is intensively investigated in two dimensions in a vicinity of the quantum critical point. For classical spins, this model has been studied numerically in [14], where it has been found that transitions on the continuous and discrete order parameters occur at different temperatures. Generally, in two-dimensional models from the same symmetry class, transitions on both order parameters occur separately in temperature or coalesce into a single transition of first order [15].

* aosorokin@gmail.com

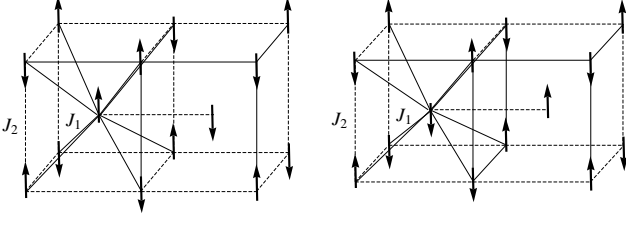


Figure 1. Exchange interactions in the ABC model. We show two configurations with opposite chirality irreducible to each other by global spin rotations and inversions.

The considered lattice models belong to the universality class with the broken $\mathbb{Z}_2 \otimes SO(2)$ symmetry being discussed above, but they are described by another functional (the $\mathbb{Z}_2 \otimes O(N)$ -model) [16]

$$F = \int d^3x \left((\partial_\mu \phi_1)^2 + (\partial_\mu \phi_2)^2 + r(\phi_1^2 + \phi_2^2) + u(\phi_1^4 + \phi_2^4) + 2w(\phi_1 \phi_2)^2 + 2v\phi_1^2 \phi_2^2 \right), \quad (2)$$

with $u > 0$, $w < 0$ and $u + v + w > 0$. For the case $N = 2$, the models (1) and (2) are equivalent in the mean-field approximation, but critical fluctuation in them are different. Nevertheless, we find a transition of a weak first order in both lattice models. Moreover, we observe the critical pseudo-exponents, which are close to the exponents of STA and helimagnets. The comparing of results is shown in table I.

II. MODELS AND METHODS

The model of an antiferromagnet on a body-centered cubic lattice (for brevity, the ABC-model) is described by the Hamiltonian

$$H = J_1 \sum_{ij} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{kl} \mathbf{S}_k \mathbf{S}_l, \quad (3)$$

where the sum ij runs over pairs of nearest spins of a lattice, and the sum kl runs over next-nearest spins (fig. 1). A spin \mathbf{S} is a classic 2-component vector, $J_1, J_2 > 0$. When $J_2 < 2J_1/3$, the ground state is two ferromagnetic sublattices interacting antiferromagnetically, and the frustration does not appear. But when $J_2 > 2J_1/3$, sublattices become antiferromagnetic. Two non-equivalent ground states are present in fig. 1.

Another model, called as the SJJ model, is

$$H = -J_1 \sum_{ij} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{kl} \mathbf{S}_k \mathbf{S}_l, \quad (4)$$

where the sum ij runs over nearest spin pairs of simple cubic lattice, and the sum kl enumerates next-nearest spin pairs in layers (fig. 2). When $J_2 < J_1/2$, the ground state is a ferromagnetic ordering. When $J_2 > J_1/2$, two type of configurations with wave-vectors $\mathbf{q} = (\pi, 0, 0)$ and

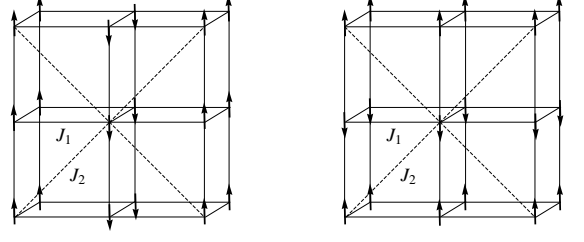


Figure 2. Exchange interactions in the SJJ model. We show two configurations with opposite chirality irreducible to each other by global spin rotations and inversions.

$\mathbf{q} = (0, \pi, 0)$ correspond to the ground state. This model is equivalent to two simple tetragonal antiferromagnetic sublattices with lattice vectors $(1, 1, 0)$, $(1, -1, 0)$ and $(0, 0, 1)$, embedded into each other and shifted relative to one another with the vector $(1, 0, 0)$. Wherein the exchange J_2 is related to an internal interaction of sublattice, and J_1 is an interaction between sublattices.

The proposed models (4) and (3) are studied by Monte Carlo simulations using the over-relaxed algorithm [17]. To define the order of a transition, we use the histogram analysis method. Thermalization is performed within $2 \cdot 10^5$ Monte Carlo steps per spin, and calculation of averages, within $3.4 \cdot 10^6$ steps. We use periodic boundary conditions and consider lattices with sizes $16 \leq L \leq 100$. The values of exchanges are chosen as $J_1 = J_2 = 1$.

The magnetic order parameter in both models is define using four sublattices

$$\mathbf{m}_i = \frac{4}{L^3} \sum_{\mathbf{x}_i} \mathbf{S}_{\mathbf{x}_i}, \quad \bar{m} = \sqrt{\frac{1}{4} \sum_{i=1}^4 \langle \mathbf{m}_i^2 \rangle}, \quad (5)$$

where \mathbf{x}_i runs over cites of the i -th sublattice, L^3 is the volume of the system (a number of spins in the ABC model is equal to $2L^3$). The chirality in the SJJ model is the following

$$k = \frac{1}{4L^3} \sum_{\mathbf{x}} (\mathbf{S}_{\mathbf{x}} - \mathbf{S}_{\mathbf{x}+\mathbf{e}_1+\mathbf{e}_2}) (\mathbf{S}_{\mathbf{x}+\mathbf{e}_1} - \mathbf{S}_{\mathbf{x}+\mathbf{e}_2}), \quad \bar{k} = \langle |k| \rangle, \quad (6)$$

with \mathbf{e}_μ is a unit vector along corresponding direction of a lattice. In the ABC model, the chiral order parameter is defined as

$$k = \frac{1}{8L^3} \sum_{\mathbf{x}} \mathbf{S}_{\mathbf{x}+\mathbf{a}} (\mathbf{S}_{\mathbf{x}} - \mathbf{S}_{\mathbf{x}+\mathbf{e}_1} - \mathbf{S}_{\mathbf{x}+\mathbf{e}_2} - \mathbf{S}_{\mathbf{x}+\mathbf{e}_3} + \mathbf{S}_{\mathbf{x}+\mathbf{e}_1+\mathbf{e}_2} + \mathbf{S}_{\mathbf{x}+\mathbf{e}_1+\mathbf{e}_3} + \mathbf{S}_{\mathbf{x}+\mathbf{e}_2+\mathbf{e}_3} - \mathbf{S}_{\mathbf{x}+\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3}), \quad (7)$$

with $\mathbf{a} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is the shift vector of antiferromagnetic sublattices.

To estimate the transition temperature on one of the order parameters $p = \bar{m}, \bar{k}$, as well as the precision of

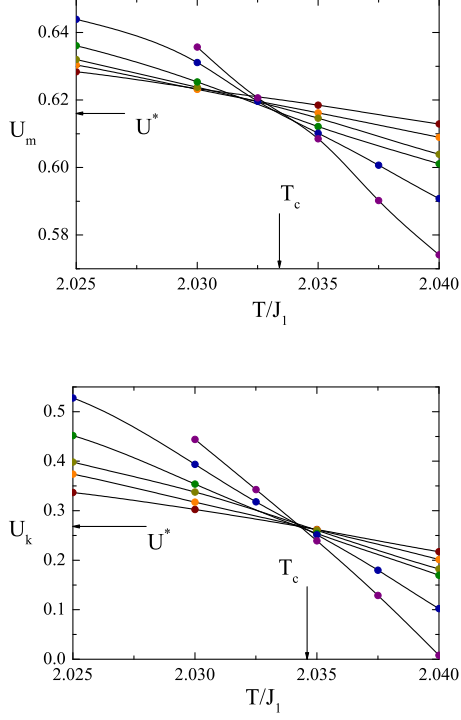


Figure 3. Estimation of the transition temperature in the SJJ model.

the estimation procedure, we use the Binder cumulant crossing method [18]

$$U_p = 1 - \frac{\langle p^4 \rangle}{3\langle p^2 \rangle^2}. \quad (8)$$

Critical exponent ν is estimated using the following cumulant [19]

$$V_p = \frac{\partial}{\partial(1/T)} \ln \langle p^2 \rangle = L^2 \left(\frac{\langle p^2 E \rangle}{\langle p^2 \rangle} - \langle E \rangle \right), \quad (9)$$

and besides, we duplicate the estimation procedure using all order parameters. The scaling relations are

$$\max \left(V_p^{(n)} \right) \sim L^{\frac{1}{\nu}}, \quad \bar{p}|_{T=T_c} \sim L^{-\frac{\beta}{\nu}}, \quad \chi_p|_{T=T_c} \sim L^{\frac{\gamma}{\nu}}, \quad (10)$$

with χ_p is susceptibility corresponding to the order parameter p [18]

$$\chi_p = \frac{L^d}{T} \left(\langle p^2 \rangle - \langle |p| \rangle^2 \right), \quad T < T_c; \\ \chi_p = \frac{L^d}{T} \langle p^2 \rangle, \quad T \geq T_c. \quad (11)$$

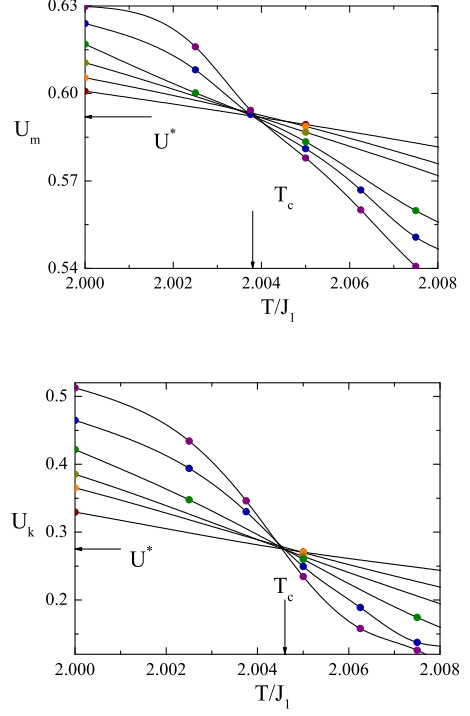


Figure 4. Estimation of the transition temperature in the ABC model.

III. RESULTS

In the SJJ model with $N = 2$, the transition temperatures on the magnetic and chiral order parameters are estimated as (fig. 3):

$$T_c^{(m)}/J_1 = 2.0334(12), \quad T_c^{(k)}/J_1 = 2.0346(10), \quad (12)$$

with the values of The Binder cumulant

$$U_m^* = 0.616(5), \quad U_k^* = 0.268(8). \quad (13)$$

Thus, within the accuracy of the results, we are dealing with a single transition. Similarly, for the ABC model we find (fig. 4)

$$T_c^{(m)}/J_1 = 2.0038(7), \quad T_c^{(k)}/J_1 = 2.0046(9), \quad (14)$$

$$U_m^* = 0.592(4), \quad U_k^* = 0.275(7). \quad (15)$$

Note that the value of the Binder cumulant at a critical point is expected to be universal depending on boundary conditions while a transition is of second order. However, for the three-dimensional XY helimagnet, the values $U_m^* = 0.623(7)$ and $U_k^* = 0.39(3)$ have been found [20], which contradict to the present results. It is more unexpectedly that the critical exponents describing the pseudo-scaling behavior of the considered models are

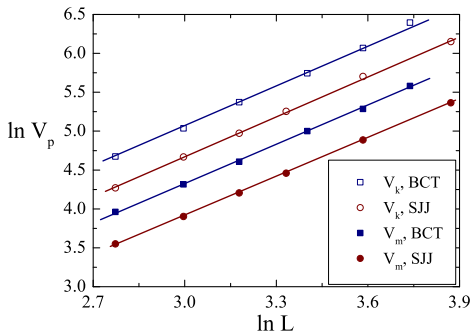


Figure 5. Estimation of the exponents ν_p using the scaling of the cumulant (9) for both models.

in agreement with the known results of STA and helimagnets. Table I shows the exponent estimations and their comparison with critical indices of other symmetry classes.

We find that the phase transition is of first order. To observe a jump of the internal energy typical for first-order transitions, we consider large lattices with $L = 80, 90, 100$. Similar sizes of a lattice have been used to determine the transition order in STA [23] and helimagnets [20]. The double-peak structure of energy distribution at the critical point indicates the presence of internal heat of a transition, it is shown in fig. 6.

IV. DISCUSSION

The $\mathbb{Z}_2 \otimes SO(2)$ symmetry, broken in a ordered phase of XY magnetic systems with a planar spin ordering, is a symmetry group acting in the spin space and related to global spin rotations and inversions. For spins with an arbitrary number of vector components, the $O(N)$ symmetry is broken down to $O(N-2)$ subgroup below a critical temperature. For the systems considered in the present work, this symmetry is broken down to $O(N-1)$ subgroup merely, and the additional \mathbb{Z}_2 factor responds to a lattice symmetry breaking. The class $\mathbb{Z}_2 \otimes O(N)/O(N-1)$ containing these lattice models and the class $O(N)/O(N-2)$ of magnets with a planar ordering become equivalent just for $N = 2$. Nonetheless, even for the case $N = 2$, the critical behavior in systems from these classes describes generally by non-equivalent models (1) and (2). Though both models exhibit a similar critical behavior, namely that a transition is of weak first order.

The model (2) includes the model (1) with $w = u - v > 0$ as a particular case. The region of the RG-flow slowdown, explaining the pseudo-scaling behavior in canted magnetic systems, resides in the sector $w > 0$. At the same time, the $\mathbb{Z}_2 \otimes O(N)/O(N-1)$ symmetry breaking scenario corresponds to the sector $w < 0$, where is no fixed point for $N \geq 2$, even complex-valued with $\text{Re } w < 0$ [16]. Therefore, a search of a RG-flow slow-

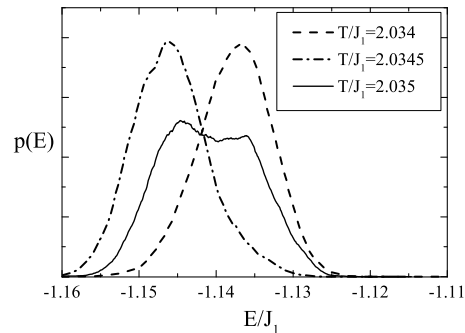


Figure 6. Internal energy distribution for $L = 90$ near the critical temperature in the SJJ model.

down region in the sector $w < 0$ must be performed independently on the known results [5, 6].

The investigations of the model (1) with $N = 2$ using non-perturbative RG [5, 6] have shown that the region of the RG-flow slowdown is wide enough and does not have a distinct center associated with a local minimum of the RG-flow, in contradistinction to the case $N = 3$. Moreover, the region includes a vicinity of the Heisenberg fixed point with $w = 0$ responding to the $O(4)$ model. It explains a variation in pseudo-exponent values observed in numerical studies and experiments (see [3] for a review). The exponents may take values close to the Kawamura's critical indices for STA [22] as well as close to the indices of the $O(4)$ model. We expect that the region of the slow RG-flow continues to the sector $w < 0$ and probably encompasses not only a vicinity of the Heisenberg point, but also a vicinity of the decoupled fixed point $w = v = 0$ responding to two non-interacting $O(2)$ models. (Fixed points of the model (2) have been found in [16], and the case $w = 0$ has been studied extensively in [24].) Such a wide region may contain trajectories, where the imitated scaling behavior is described by exponents close to the Kawamura's results, but without the pseudo-universality.

When w is sufficiently small, it is possible to explain the observed pseudo-universality by another way, associated with a tricritical behavior. Such a possibility has been discussed for STA in [25]. In table I, we show the mean-field values of the tricritical exponents, which are close to the exponents of systems with the breaking $\mathbb{Z}_2 \otimes SO(2)$ symmetry. While the term $w(\phi_1 \phi_2)^2$ is small, the scaling is determined by terms like $w_6(\phi_1 \phi_2)^3$. The later terms are inessential at a critical point, but they can lead to crossover between a tricritical and critical behaviors, discernible in simulations on finite-size lattices or at some distance on temperature from a critical point. Note that such a crossover have been observed in a similar model in two dimensions [26].

One can consider one more possibility associated with an approximation of first-order transition singularities in the finite-size-scaling theory. In table I, we show also

Table I. Comparison of the (pseudo) critical exponents obtained in the present work (marked as [*]) with known exponents of other universality classes. Notations: Ising — the Ising model, Ferro — ferromagnetic or the $O(N)$ model, Helix — helimagnets, STA — antiferromagnet on a stacked-triangular lattice, FSS — typical exponents for a first-order transition in the finite-size-scaling theory.

Class G/H	Model	Ref.	ν	ν_k	β	$\beta_k/2$	γ	$\gamma_k + \beta_k$
\mathbb{Z}_2	Ising	[21]	0.630		0.327		1.236	
$SO(2)$	Ferro	[21]	0.671		0.348		1.317	
$SO(3)/SO(2)$	Ferro	[21]	0.706		0.365		1.388	
$SO(4)/SO(3)$	Ferro	[21]	0.75		0.39		1.47	
Tricritical	Mean-field		0.5	0.5	0.25	0.25	1.00	1.00
First order	FSS		0.33	0.33	0	0	1.00	1.00
$\mathbb{Z}_2 \otimes SO(2)$	Helix	[20]	0.55	0.56	0.25	0.21	1.16	1.29
$\mathbb{Z}_2 \otimes SO(2)$	STA	[22]	0.54	0.55	0.25	0.23	1.13	1.22
$\mathbb{Z}_2 \otimes SO(2)$	SJJ	[*]	0.565(8)	0.572(10)	0.260(6)	0.251(8)	1.18(4)	1.22(5)
$\mathbb{Z}_2 \otimes SO(2)$	ABC	[*]	0.568(10)	0.571(9)	0.262(7)	0.258(10)	1.18(5)	1.20(8)

typical "exponents" for a first-order transition, but they are disagreement with the exponents of the considered models. Apparently, such an explanation is not applicable to the weak first-order or "almost second-order" transitions.

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